CALCULATING A POTENTIAL OF MEAN FORCE (PMF) SCORE OF A PROTEIN-LIGAND COMPLEX

ABSTRACT OF THE DISCLOSURE

In one embodiment, a system for calculating a potential of mean force (PMF) score of a protein-ligand complex includes a repulsion-term module that accesses one or more parameters useable to calculate a repulsion term useable to calculate a PMF of a protein-ligand atom pair in the protein-ligand complex. The one or more parameters correspond to an atom-pair type of the protein-ligand atom pair. The repulsion-term module uses the one or more accessed parameters to calculate the repulsion term useable to calculate the PMF of the protein-ligand atom pair. Th repulsion-term module communicates the calculated repulsion term for calculation of the PMF score of the protein-ligand complex.